Correlated projection operator approach to non-Markovian dynamics in spin baths

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The dynamics of an open quantum system is usually studied by performing a weak-coupling and weak-correlation expansion in the system-bath interaction. For systems exhibiting strong couplings and highly non-Markovian behavior this approach is not justified. We apply a recently proposed correlated projection superoperator technique to the model of a central spin coupled to a spin bath via full Heisenberg interaction. Analytical solutions to both the Nakajima-Zwanzig and the time-convolutionless master equation are determined and compared with the results of the exact solution. The correlated projection operator technique significantly improves the standard methods and can be applied to many physical problems such as the hyperfine interaction in a quantum dot.

I. INTRODUCTION

Some of the key features in the dynamics of open quantum systems [1] are phenomena such as relaxation, decoherence and the buildup of correlations and entanglement due to the interaction of the open system with its environment. This behavior is generic in the sense that it is observable for many different kinds of environments and microscopic interactions. For many physical systems it is justified to assume that the coupling to the environment is weak (Born approximation) or that correlations in the bath decay quickly with respect to the typical timescale of the system's dynamics (Markov approximation). In this case it is often possible to construct a generator for the dynamics which is in Lindblad form [2, 3].

In general, however, memory effects in the bath cannot be neglected and the Markov assumption is not applicable any more. Such systems are said to exhibit non-Markovian behavior. This can be due to strong system-environment couplings [4, 5], correlations and entanglement in the initial state [6, 7], finite reservoirs [8, 9], or due to coupling to environments at low temperatures or to spin baths [10, 11, 12]. Also, heat transport in nanostructures [13] has been shown to exhibit non-Markovian behavior.

A powerful tool for dealing with such systems is provided by the projection operator techniques [14, 15] which have been introduced by Nakajima [16], Zwanzig [17] and Mori [18]. These techniques are based on the introduction of a projection superoperator $\mathcal{P}$ which acts on the density operator ρ of the total system and projects onto the so-called relevant part $\mathcal{P}\rho$. The latter represents a certain approximation of ρ, and this procedure leads to a simplified effective description of the dynamics through a reduced set of relevant variables. Stated differently, the projection $\mathcal{P}$ expresses the elimination of certain degrees of freedom which are considered negligible for the treatment of the open system's dynamics.

Here, we will consider two different approaches which both lead to a closed equation for the dynamics of the relevant part of ρ. The first one leads to the Nakajima-Zwanzig equation [16, 17], an integrodifferential master equation for $\mathcal{P}\rho$ containing a memory kernel. The second approach eliminates the integration over the system's history and leads to the time-convolutionless master equation which is local in time, but involves a time-dependent generator [19, 20, 21, 22, 23, 24]. In both cases the resulting master equation is used as a starting point for a systematic expansion in powers of the system-environment interaction.

Usually the projector is chosen such that $\mathcal{P}\rho = (\mathrm{tr}_E\rho) \otimes \rho_0 = \rho_S \otimes \rho_0$, where ρ_0 is some fixed environmental state, e.g. a thermal equilibrium state, and where tr_E denotes the partial trace over the environment. The superoperator $\mathcal{P}$ projects the total state ρ onto a tensor-product state, i.e., onto a state without any statistical correlations between the open system and its environment. If correlations remain small, this ansatz is justified and the perturbation expansion is usually carried out only to leading order in the perturbation (Born approximation). However, for many physical systems exhibiting strong correlations, the Born approximation might be inadequate such that one also has to take into account higher orders of the expansion. The calculation of higher orders is limited by the increase of mathematical complexity, though, and furthermore, the expansion may not converge uniformly in time, such that higher orders may diverge on longer timescales [25].

A different strategy for taking strong correlations into account is to introduce a superoperator $\mathcal{P}$ that projects onto a correlated system-environment state, i.e., onto a state that contains certain statistical correlations between the open system and its environment [26, 27, 28, 29, 30, 31, 32]. We will refer to such $\mathcal{P}$ as a correlated projection superoperator. In the present article we will discuss in detail the application of the correlated projection operator method to a two level system interacting

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with a spin bath. This system is particularly interesting since it models the hyperfine interaction of an electron confined to a quantum dot with its surrounding nuclei [11].

We organize this paper as follows. In Sec. II we review the standard projection operator technique and formulate the Nakajima-Zwanzig as well as the time-convolutionless master equation. Also, we briefly recapitulate how to extend the technique to correlated projection superoperators. In Sec. III we apply this method to a simple spin-bath model and construct projectors on the basis of symmetry considerations that vastly improve the performance of the projection operator technique. We compare the resulting solutions of the Nakajima-Zwanzig and the time-convolutionless master equation in second order to an exact solution of the model. Discussion and conclusions are then provided in Sec. IV.

II. PROJECTION OPERATOR TECHNIQUES

In general, one considers an open system S which is coupled to some environment E. The accordant Hilbert spaces are denotes by $\mathcal{H}_S$ and $\mathcal{H}_E$, respectively, and the state space of the total system is given by the product $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$. The Hamiltonian of the total system is denoted by $H = H_0 + H_I$, where H_0 is the unperturbed part of the Hamiltonian and H_I represents the interaction between system and bath. A general state of the total system is given by a density matrix ρ. The partial traces over the system S and the environment E are denoted by tr_S and tr_E, respectively. The reduced density matrix of the open system is thus given by $\rho_S = \mathrm{tr}_E \rho$.

A. The standard projection superoperator

The starting point of the projection operator techniques is the introduction of a superoperator $\mathcal{P}$ which acts on the total system's density matrix, and which is defined by

$$\mathcal{P}\rho = (\mathrm{tr}_E \rho) \otimes \rho_0, \tag{1}$$

where ρ_0 is some fixed state of the environment. The map $\mathcal{P}$ satisfies the condition of a projector, namely $\mathcal{P}^2 = \mathcal{P}$, and is therefore referred to as a projection superoperator, being a map acting on operators. The complementary map is defined via $\mathcal{Q} = I - \mathcal{P}$, where I denotes the identity. Note that $\mathcal{P}\rho$ contains all information about the open system in the sense that for the expectation value of any observable $\mathcal{O}_S$ of the open system the relation $\mathrm{tr}\{\mathcal{O}_S \rho\} = \mathrm{tr}\{\mathcal{O}_S \mathcal{P}\rho\}$ holds.

B. Nakajima-Zwanzig equation

Starting from the von Neumann equation in the interaction picture with respect to H_0,

$$\frac{d}{dt}\rho(t) = -i[H_I(t), \rho(t)] \equiv \mathcal{L}(t)\rho(t), \tag{2}$$

one can derive a closed equation for the projection $\mathcal{P}\rho(t)$ by inserting $\mathcal{P}$ and $\mathcal{Q}$ in front of ρ on both sides,

$$\frac{d}{dt}\mathcal{P}\rho(t) = \int_0^t dt_1\, \mathcal{K}(t, t_1)\mathcal{P}\rho(t_1). \tag{3}$$

The superoperator

$$\mathcal{K}(t, t_1) = \mathcal{P}\mathcal{L}(t)\, \mathrm{T}\exp\left[\int_{t_1}^t dt_2\, \mathcal{Q}\mathcal{L}(t_2)\right]\mathcal{Q}\mathcal{L}(t_1)\mathcal{P} \tag{4}$$

is referred to as the memory kernel or the self-energy, and the operator T denotes chronological time-ordering. Eq. (3) is called the Nakajima-Zwanzig (NZ) equation and describes non-Markovian behavior of the total system through the memory kernel (4). In general, there is an additional term proportional to $\mathcal{Q}\rho(0)$ on the right-hand side of the NZ equation which we have omitted here for simplicity, supposing an initial state that satisfies $\mathcal{P}\rho(0) = \rho(0)$. Since $\mathcal{K}(t, t_1)$ is usually a very complicated operator, it is customary to perform a perturbation expansion in powers of H_I. Under the condition

$$\mathcal{P}\mathcal{L}(t)\mathcal{P} = 0 \tag{5}$$

the lowest-order contribution is given by the second order,

$$\frac{d}{dt}\mathcal{P}\rho(t) = \int_0^t dt_1 \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{P}\rho(t_1), \tag{6}$$

and higher orders are obtained by expanding the time-ordered exponential of the memory kernel (4).

C. Time-convolutionless master equation

An alternative way of deriving an exact master equation for the relevant part of ρ is to remove the dependence of the system's dynamics on the full history of the system and to formulate a time-local equation of motion, which is given by

$$\frac{d}{dt}\mathcal{P}\rho(t) = \mathcal{K}(t)\mathcal{P}\rho(t). \tag{7}$$

This equation is called the time-convolutionless (TCL) master equation, and $\mathcal{K}(t)$ is a time-dependent superoperator, which is referred to as the TCL generator. As for the NZ equation, in general there is also a term proportional to $\mathcal{Q}\rho(0)$ on the right-hand side of Eq. (7), which vanishes provided one chooses a factorized initial state.

Like for the NZ equation one can carry out a perturbation expansion of the TCL generator in powers of H_I. The various orders of this expansion can be expressed through the ordered cumulants [33, 34, 35, 36] of the Liouville superoperator $\mathcal{L}(t)$. The second-order contribution reads

$$\mathcal{K}_2(t) = \int_0^t dt_1 \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{P}, \qquad (8)$$

such that the second-order TCL master equation takes the form

$$\frac{d}{dt}\mathcal{P}\rho(t) = \int_0^t dt_1 \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{P}\rho(t), \qquad (9)$$

which should be contrasted to the second-order NZ equation (6). One can formulate a simple set of rules that enable one to write down immediately these expressions and the corresponding expressions for all higher orders [1]. The TCL technique has been applied to many physical systems. Examples, which include the determination of higher orders of the expansion, are the damped Jaynes-Cummings model [37], quantum Brownian motion and the spin-boson model [38], the spin-star model [25], relaxation processes in structured reservoirs [27], and the dynamics of the atom laser [39]. Applications of the TCL method to systems relevant for quantum information processing may be found in [40, 41]. Recently, the performance of the TCL approach has been studied for the model of a qubit coupled to a spin bath via Ising interaction [42], and for a general open system coupled to a bath through pure phase noise [43].

We emphasize at this point that the TCL master equation describes non-Markovian dynamics although it is local in time. All memory effects are taken into account by the explicit time-dependence of the TCL generator. It should also be pointed out that both the NZ equation (3) and the TCL equation (7) are exact in the sense that they are equivalent to the equation of motion gained from the full system Hamiltonian.

It is important to realize that the NZ and the TCL techniques lead to equations of motion with entirely different structures. Therefore, also the mathematical structure of their solutions are quite different in any given order [44]. It turns out that in many cases the degree of accuracy obtained by both methods is of the same order of magnitude. In these cases the TCL approach is of course to be preferred because it is technically much simpler to deal with.

D. Correlated projection superoperators

The performance of the projection operator techniques depends on the properties of the microscopic model under study, in particular on the structure of the environmental correlation functions. However, it also depends strongly on the choice of the superoperator $\mathcal{P}$. Several extensions of the standard projection (1) and modifications of the expansion technique have been proposed in the literature (see, e.g., [45, 46, 47]).

A characteristic feature of the projection defined by Eq. (1) is given by the fact that it projects any state ρ onto a tensor product $\rho_S \otimes \rho_0$ that describes a state without statistical correlations between the system and its environment. This is not the only possible choice. In fact, a general class of projection superoperators can be represented as follows,

$$\mathcal{P}\rho = \sum_i \mathrm{tr}_E\{A_i\rho\} \otimes B_i, \qquad (10)$$

where $\{A_i\}$ and $\{B_i\}$ are two sets of linear independent Hermitian operators on $\mathcal{H}_E$ satisfying the relations

$$\mathrm{tr}_E\{B_i A_j\} = \delta_{ij}, \qquad (11)$$

$$\sum_i (\mathrm{tr}_E B_i) A_i = I_E, \qquad (12)$$

$$\sum_i A_i^T \otimes B_i \geq 0. \qquad (13)$$

The map defined by Eq. (10) projects in general onto correlated (non-factorizing) system-environment states and may thus be referred to as a correlated projection superoperator. It can be shown [26] that Eq. (10) represents the most general form of such a correlated projection superoperator under certain natural physical conditions. These conditions demand that $\mathcal{P}$ is a completely positive and trace preserving map (quantum channel) that operates on the environmental variables. Equation (11) guarantees that $\mathcal{P}$ is a projection superoperator, Eq. (12) ensures that $\mathcal{P}$ preserves the trace (normalization), while Eq. (13) is equivalent to the condition of complete positivity (T denotes the transposition). We remark that the class of projections defined by Eq. (10) yields a natural generalization of the Lindblad equation to the regime of strong non-Markovian quantum dynamics [26, 28].

A typical example for a correlated projection that is relevant for the present paper is obtained by the choice

$$A_i = \Pi_i, \qquad B_i = \frac{1}{N_i}\Pi_i, \qquad N_i = \mathrm{tr}_E \Pi_i, \qquad (14)$$

where the Π_i are ordinary projection operators on $\mathcal{H}_E$ which form an orthogonal decomposition of the unit operator:

$$\Pi_i \Pi_j = \delta_{ij}\Pi_j, \qquad \Pi_i^\dagger = \Pi_i, \qquad \sum_i \Pi_i = I_E. \qquad (15)$$

One easily checks that with this choice all conditions formulated above are indeed satisfied. Further examples are discussed in Refs. [26, 27, 28, 31, 32].

As mentioned already in Sec. II C, a homogeneous NZ or TCL equation of motion presupposes a tensor product initial state if one uses the standard projection superoperator (1). However, this is no longer true for the correlated projection defined by Eq. (10). In fact, the general

condition for the absence of an inhomogeneous term in the NZ equation (3) or the TCL equation (7) is given by $\mathcal{P}\rho(0) = \rho(0)$. According to Eq. (10) this condition does *not* require that $\rho(0)$ be a factorized state. Hence, a great advantage of the correlated projection superoperators is given by the fact that they allow the treatment of correlated initial states by means of a homogeneous NZ or TCL equation [26, 48].

Once $\mathcal{P}$ is chosen, the dynamics of the open system is uniquely determined by the dynamical variables

$$\rho_i(t) = \text{tr}_E\{A_i\rho(t)\}. \tag{16}$$

The connection to the reduced density is simply given by

$$\rho_S(t) = \sum_i \rho_i(t), \tag{17}$$

and the normalization condition reads

$$\text{tr}_S\,\rho_S(t) = \sum_i \text{tr}_S\,\rho_i(t) = 1. \tag{18}$$

The reduced density matrix is hence uniquely determined by a set of (unnormalized) operators $\rho_i(t)$. With the help of the NZ equation (3) one finds that the dynamics of these operators is governed by a coupled system of integrodifferential equations,

$$\frac{d}{dt}\rho_i(t) = \sum_j \int_0^t dt_1\, \mathcal{K}_{ij}(t,t_1)\rho_j(t_1), \tag{19}$$

where the superoperators $\mathcal{K}_{ij}(t,t_1)$ are defined through their action on an arbitrary system operator $\mathcal{O}_S$,

$$\mathcal{K}_{ij}(t,t_1)\mathcal{O}_S \equiv \text{tr}_E\left\{A_i\mathcal{K}(t,t_1)(\mathcal{O}_S \otimes B_j)\right\}. \tag{20}$$

On the other hand, the TCL equation (7) leads to a coupled system of time-local differential equations,

$$\frac{d}{dt}\rho_i(t) = \sum_j \mathcal{K}_{ij}(t)\rho_j(t), \tag{21}$$

with superoperators defined by

$$\mathcal{K}_{ij}(t)\mathcal{O}_S \equiv \text{tr}_E\left\{A_i\mathcal{K}(t)(\mathcal{O}_S \otimes B_j)\right\}. \tag{22}$$

A crucial step for a successful applications of the correlated projection operator technique is the construction of an appropriate projection superoperator $\mathcal{P}$. A useful strategy for this construction is to take into account the known conserved quantities of the model under study. Let us suppose that C is a such conserved quantity. Then a good choice for $\mathcal{P}$ is a projection that leaves invariant the expectation values of C, i.e., $\text{tr}\{C\rho\} = \text{tr}\{C\mathcal{P}\rho\}$. Requiring this to hold for all states ρ we get the condition

$$\mathcal{P}^\dagger C = C, \tag{23}$$

where $\mathcal{P}^\dagger$ denotes the adjoint of $\mathcal{P}$ with respect to the Hilbert-Schmidt scalar product [48]. This equation represents a condition for the projection superoperator $\mathcal{P}$

on the basis of a known conserved quantity of the underlying model. It ensures that the projection superoperator leaves invariant this quantity and that the effective description respects the corresponding conservation law [31, 32].

III. APPLICATION TO A SPIN BATH

A. Description of the model

We want to apply the correlated projection operator formalism to a spin-bath model, which is defined by the Hamiltonian

$$H = \frac{\omega_0}{2}\sigma_3 + \sum_{k=1}^N A_k \boldsymbol{\sigma} \cdot \boldsymbol{\sigma}^{(k)}. \tag{24}$$

The central spin, representing the open system, has an energy splitting ω_0 and is coupled to the k-th bath spin via the coupling constant A_k. Here, $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}^{(k)}$ are the Pauli operators of the central spin and of the k-th bath spin, respectively.
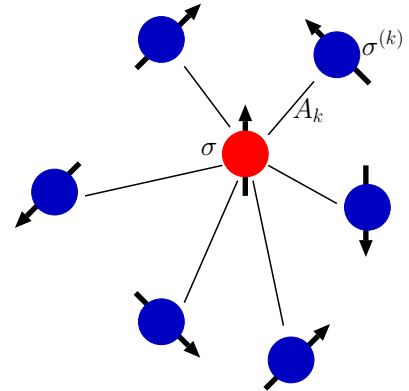

FIG. 1: (Color online) Illustration of the model with Hamiltonian (24). A central spin $\boldsymbol{\sigma}$ interacts with a bath of N spins $\boldsymbol{\sigma}^{(k)}$ through the coupling constants A_k.

In the following we will restrict ourselves to initial states of the form

$$\rho(0) = \rho_S(0) \otimes \frac{1}{2^N}I_E, \tag{25}$$

where I_E is the unit matrix in the state space of the spin bath. Initially the bath is thus in a completely unpolarized (infinite temperature) state. This choice is made here only for simplicity; the present method also allows the treatment of polarized bath states and of correlated initial states.

Our aim is to illustrate the TCL and the NZ expansion for a correlated projection superoperator. To compare the results with the exact solution of the full von Neumann equation corresponding to the Hamiltonian (24)

we take the coupling constants to be independent of k, i.e., $A_k = A$. The model can then be solved analytically as follows. First one notes that the 3-component of the angular momentum of the total system,

$$J_3^{\text{tot}} = \frac{1}{2}\sigma_3 + J_3, \tag{26}$$

is conserved under the time-evolution given by the Hamiltonian (24). Here, J_3 denotes the 3-component of the angular momentum of the bath which is defined by

$$\boldsymbol{J} = \frac{1}{2}\sum_k \boldsymbol{\sigma}^{(k)}. \tag{27}$$

For $A_k = A$, also the square $\boldsymbol{J}^2$ of the bath angular momentum is conserved. We introduce basis states $|j, m\rangle$ which are defined as simultaneous eigenstates of $\boldsymbol{J}^2$ and J_3 [49]. If N is even, j takes on the values $j = 0, 1, 2, \ldots, \frac{N}{2}$, while $j = \frac{1}{2}, \frac{3}{2}, \ldots, \frac{N}{2}$ for odd N. For a given value of j, the quantum number m takes on the values $m = -j, -j+1, \ldots, +j$.

With the help of the conserved quantities one easily solves the time-dependent Schrödinger equation, employing the fact that the two-dimensional subspaces spanned by the states $|+\rangle \otimes |j, m\rangle$ and $|-\rangle \otimes |j, m+1\rangle$ are invariant under the time-evolution. Here, the states $|\pm\rangle$ denote the eigenstates of the central spin, $\sigma_3|\pm\rangle = \pm|\pm\rangle$. We further introduce the quantities

$$p(j) = \frac{2j+1}{2^N}N_j, \tag{28}$$

where

$$N_j = \binom{N}{\frac{N}{2}+j} - \binom{N}{\frac{N}{2}+j+1} \tag{29}$$

represents the number of times the angular momentum j appears in the decomposition of the bath Hilbert space into irreducible subspaces of the rotation group. Hence, $p(j)$ may be interpreted as the probability of finding a certain angular momentum j in the initial state of the bath. Finally, we define the frequencies

$$\Omega_\pm(m) = \pm\omega_0 + 4A(\pm m + 1/2),$$
$$\mu_\pm(j, m) = \sqrt{\frac{\Omega_\pm^2(m)}{4} + 4A^2[j(j+1) - m(m \pm 1)]}.$$

With the help of these definitions the upper state population of the central spin can be written as

$$\begin{aligned} P_+(t) &= \langle +|\rho_S(t)|+\rangle \\ &= \sum_{jm} \frac{p(j)}{2j+1}\Big[\cos^2[\mu_+(j, m)t] \\ &\quad + \frac{\Omega_+^2(m)}{4\mu_+^2(j, m)}\sin^2[\mu_+(j, m)t]\Big], \end{aligned} \tag{30}$$

where we have used for simplicity the initial condition $P_+(0) = 1$. The lower state population is found from

$P_-(t) = \langle -|\rho_S(t)|-\rangle = 1 - P_+(t)$. The coherence of the central spin is determined by the formula

$$\begin{aligned} \rho_{+-}(t) &= \langle +|\rho_S(t)|-\rangle \\ &= \rho_{+-}(0)\sum_{jm}\frac{p(j)e^{i\omega_0 t}}{2j+1} \\ &\quad \times \left[\cos[\mu_+(j, m)t] - \frac{i\Omega_+(m)}{2\mu_+(j, m)}\sin[\mu_+(j, m)t]\right] \\ &\quad \times \left[\cos[\mu_-(j, m)t] + \frac{i\Omega_-(m)}{2\mu_-(j, m)}\sin[\mu_-(j, m)t]\right]. \end{aligned}$$

B. Correlated projection operators

According to Sec. II D, a good candidate for a correlated projection superoperator is a map that does not change the expectation values of the known conserved quantities. We start by using a projection superoperator $\mathcal{P}$ that leaves invariant the 3-component of the total angular momentum, i.e., that satisfies [see Eq. (23)]

$$\mathcal{P}^\dagger J_3^{\text{tot}} = J_3^{\text{tot}}, \tag{31}$$

We define bath operators Π_m which project onto the subspace spanned by the eigenstates of J_3 corresponding to the eigenvalue $m = -\frac{N}{2}, \ldots, +\frac{N}{2}$. An appropriate projection operator with the property (31) is then given by

$$\mathcal{P}\rho = \sum_m \text{tr}_E\{\Pi_m\rho\} \otimes \frac{1}{N_m}\Pi_m \equiv \sum_m \rho_m \otimes \frac{1}{N_m}\Pi_m, \tag{32}$$

where the number

$$N_m = \text{tr}_E\Pi_m = \binom{N}{\frac{N}{2}+m} \tag{33}$$

represents the degree of degeneracy of the eigenvalue m of J_3. One can easily check that this projection operator satisfies all conditions formulated in Sec. II D.

The state of the central spin is thus determined by the set of densities $\rho_m(t)$. The projection $\mathcal{P}\rho$ represents a correlated system-environment state in which each ρ_m is correlated with the bath state Π_m/N_m which describes a state of maximal entropy under the constraint of a given value m for the 3-component of the angular momentum. According to Eq. (17) the reduced density matrix is obtained from

$$\rho_S(t) = \sum_m \rho_m(t), \tag{34}$$

and its normalization condition reads

$$\text{tr}_S \rho_S(t) = \sum_m \text{tr}_S \rho_m(t) = 1. \tag{35}$$

Finally, the matrix elements of the $\rho_m(t)$ are defined by

$$P_\pm^m(t) = \langle \pm|\rho_m(t)|\pm\rangle, \tag{36}$$
$$\rho_{+-}^m(t) = \langle +|\rho_m(t)|-\rangle. \tag{37}$$

It should be emphasized that the above procedure is also applicable if the coupling constants A_k are not equal to each other, since J_3^{tot} is then still a conserved quantity. We remark that the standard procedure with a projection operator of the form of Eq. (1) with $\rho_0 = 2^{-N} I_E$ would give $\mathcal{P}^\dagger J_3^{\text{tot}} = \frac{1}{2}\sigma_3$.

1. Interaction Hamiltonian

We write the Hamiltonian (24) in the form $H = H_0 + H_I$, where

$$H_0 = \frac{\omega_0}{2}\sigma_3 + 2A\sigma_3 J_3 \tag{38}$$

is regarded as the unperturbed part and

$$H_I = 2A(\sigma_+ J_- + \sigma_- J_+) \tag{39}$$

as the interaction Hamiltonian. Note that the unperturbed Hamiltonian H_0 is not a sum of free Hamiltonian operators for system and environment, and that the perturbation Hamiltonian contains only the flip-flop part of the interaction, which describes the flip of the central spin accompanied by a back-flip of one of the bath spins.

We transform to the interaction picture with respect to H_0 which leads to the interaction Hamiltonian

$$H_I(t) = 2A e^{i(\omega_0 - 2A)t}\sigma_+ J_- e^{4iAJ_3 t} + \text{H.c.}$$

We will always represent our results in the interaction picture with respect to the Hamiltonian $\frac{\omega_0}{2}\sigma_3$, i.e. in the rotating frame of the central spin. The results in the interaction picture relative to H_0 are transformed back to the rotating frame of the central spin through the prescription

$$\rho_m(t) \longrightarrow e^{-2iAm\sigma_3 t}\rho_m(t)e^{+2iAm\sigma_3 t}. \tag{40}$$

Obviously, this back-transformation leaves the populations $P_\pm^m(t)$ unchanged, while the coherences pick up a phase factor,

$$\rho_{+-}^m(t) \longrightarrow e^{-4iAmt}\rho_{+-}^m(t). \tag{41}$$

2. Master equation

For the projection defined by Eq. (32) the NZ master equation (19) takes the following form in second order,

$$\frac{d}{dt}\rho_m(t) = -\sum_{m'}\int_0^t dt_1$$
$$\times \ \text{tr}_E\left\{\Pi_m\left[H_I(t),\left[H_I(t_1),\rho_{m'}(t_1)\otimes\frac{1}{N_{m'}}\Pi_{m'}\right]\right]\right\}.$$

The right-hand side of this equation is easily calculated to yield [50]

$$\frac{d}{dt}\rho_m(t) = 4A^2\int_0^t dt_1$$
$$\times\left[\sigma_+\rho_{m+1}(t_1)\sigma_-\left(\frac{N}{2}+m+1\right)2\cos[\Omega_+(m)(t-t_1)]\right.$$
$$+\sigma_-\rho_{m-1}(t_1)\sigma_+\left(\frac{N}{2}-m+1\right)2\cos[\Omega_-(m)(t-t_1)]$$
$$-\sigma_+\sigma_-\rho_m(t_1)\left(\frac{N}{2}-m\right)e^{i\Omega_+(m)(t-t_1)}$$
$$-\sigma_-\sigma_+\rho_m(t_1)\left(\frac{N}{2}+m\right)e^{i\Omega_-(m)(t-t_1)}$$
$$-\rho_m(t_1)\sigma_+\sigma_-\left(\frac{N}{2}-m\right)e^{-i\Omega_+(m)(t-t_1)}$$
$$\left.-\rho_m(t_1)\sigma_-\sigma_+\left(\frac{N}{2}+m\right)e^{-i\Omega_-(m)(t-t_1)}\right]. \tag{42}$$

One easily checks that this master equation preserves the Hermiticity and the trace of the reduced density matrix $\rho_S(t)$ which is determined by Eq. (34). Note that the dynamics couple the densities $\rho_m(t)$ to $\rho_{m\pm1}(t)$. The corresponding second-order TCL master equation Eq. (21) is obtained from Eq. (42) by just replacing $\rho_m(t_1)$ by $\rho_m(t)$ on the right-hand side.

3. Coherences

The coherence of the central spin is given by the sum of the coherences of the ρ_m,

$$\rho_{+-}(t) = \sum_m \rho_{+-}^m(t). \tag{43}$$

From the initial condition (25) we find that

$$\rho_{+-}^m(0) = \frac{N_m}{2^N}\rho_{+-}(0). \tag{44}$$

The dynamics of the coherences $\rho_{+-}^m(t)$ is determined by the master equation (42) which leads to

$$\frac{d}{dt}\rho_{+-}^m(t) = -\int_0^t dt_1\left[B_+(m)e^{i\Omega_+(m)(t-t_1)}\right.$$
$$\left.+B_-(m)e^{-i\Omega_-(m)(t-t_1)}\right]\rho_{+-}^m(t_1), \tag{45}$$

where

$$B_\pm(m) = 4A^2\left(\frac{N}{2}\mp m\right). \tag{46}$$

Note that the dynamics does not couple the different components $\rho_{+-}^m(t)$. The integrodifferential equation (45) can now be solved with the help of a Laplace transformation. The corresponding TCL equation is obtained from Eq. (45) by replacing $\rho_{+-}^m(t_1)$ by $\rho_{+-}^m(t)$ on the right-hand side. Solving the resulting equation yields

$$\rho_{+-}(t) = \rho_{+-}(0)\sum_m\frac{N_m}{2^N}\exp\left[-4iAmt-\Lambda_m^{\text{coh}}(t)\right], \tag{47}$$

where

$$\Lambda_m^{\mathrm{coh}}(t) = \frac{B_+(m)}{\Omega_+^2(m)}\left[1 - e^{i\Omega_+(m)t}\right]$$
$$+ \frac{B_-(m)}{\Omega_-^2(m)}\left[1 - e^{-i\Omega_-(m)t}\right]$$
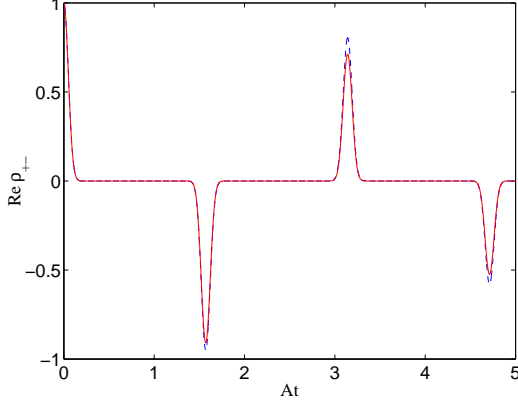$$+ i\left[\frac{B_+(m)}{\Omega_+(m)} - \frac{B_-(m)}{\Omega_-(m)}\right]t. \qquad (48)$$

FIG. 2: (Color online) Coherence of the central spin. Continuous line: Exact solution. Dashed line: Second-order NZ approximation. Parameters: $N = 101$ and $\alpha = 0.1$.
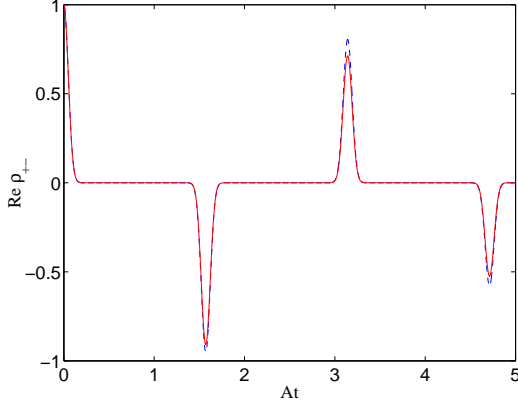

FIG. 3: (Color online) Coherence of the central spin. Continuous line: Exact solution. Dashed line: Second-order TCL approximation. Parameters: $N = 101$ and $\alpha = 0.1$.

The comparison with the exact solution shows that both methods correspond essentially to an expansion in the dimensionless quantity

$$\alpha = \frac{2AN}{\omega_0}. \qquad (49)$$

We compare the results of the NZ and the TCL method with the exact solution in Figs. 2 and 3, where the coherence is normalized such that $\rho_{+-}(0) = 1$. Both the NZ

and the TCL equation reproduce the exact solution very well in the perturbative regime. Moreover, both are capable of describing the position, the height and the width of the partial revivals of the coherence, which appear because of the finite size of the bath and the associated finite recurrence times. For large integration times, only the positions and the width of the revivals are reproduced correctly (see Fig. 4). We note that the NZ and the TCL method yield nearly identical results; they are hardly distinguishable on the scale of the shown figures.
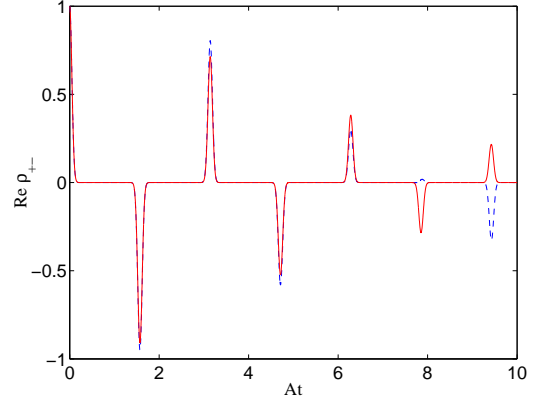

FIG. 4: (Color online) Coherence of the central spin. Continuous line: Exact solution. Dashed line: Second-order TCL approximation. Parameters: $N = 101$ and $\alpha = 0.1$.

4. Populations

The populations are given by

$$P_\pm(t) = \sum_m P_\pm^m(t). \qquad (50)$$

The initial condition (25) now yields

$$P_+^m(0) = \frac{N_m}{2^N}, \qquad P_-^m(0) = 0. \qquad (51)$$

The master equation (42) leads to

$$\frac{d}{dt}P_+^m(t) = 8A^2\int_0^t dt_1$$
$$\times \left[\left(\frac{N}{2} + m + 1\right)\cos[\Omega_+(m)(t - t_1)]P_-^{m+1}(t_1)\right.$$
$$\left. - \left(\frac{N}{2} - m\right)\cos[\Omega_+(m)(t - t_1)]P_+^m(t_1)\right], \qquad (52)$$

and

$$\frac{d}{dt}P_-^m(t) = 8A^2\int_0^t dt_1$$
$$\times \left[\left(\frac{N}{2} - m + 1\right)\cos[\Omega_-(m)(t - t_1)]P_+^{m-1}(t_1)\right.$$
$$\left. - \left(\frac{N}{2} + m\right)\cos[\Omega_-(m)(t - t_1)]P_-^m(t_1)\right]. \qquad (53)$$

Note that, in contrast to the coherences, this equation does couple different components $P_\pm^m$. However, the solution can still be constructed by noting that

$$\frac{d}{dt}\left[P_+^m(t) + P_-^{m+1}(t)\right] = 0. \qquad (54)$$

With the help of this equation one shows that the total angular momentum J_3^{tot} is exactly conserved under the dynamics given by the master equation. Namely, we deduce from Eq. (54) that

$$\frac{d}{dt}\text{tr}\left\{J_3^{\text{tot}}\mathcal{P}\rho(t)\right\}$$
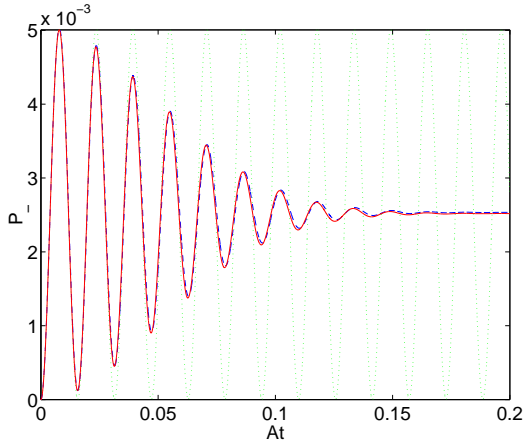$$= \frac{d}{dt}\sum_m \left(\frac{1}{2} + m\right)\left[P_+^m(t) + P_-^{m+1}(t)\right] = 0. \quad (55)$$

FIG. 5: (Color online) Population of the central spin according to the exact solution (continuous line), and to the second-order TCL approximations using the correlated projection (broken line) and the standard product-state projection (dotted line). Parameters: $N = 101$ and $\alpha = 0.5$.

Equation (54) is used to eliminate P_-^{m+1} from the right-hand side of Eq. (52) to get a closed equation for P_+^m which can again be solved with the help of a Laplace transformation. The corresponding TCL equations are solved in a similar manner yielding

$$P_+(t) = \sum_m \frac{N_m}{2^N}\left[\frac{\frac{N}{2} + m + 1}{N + 1} + \frac{\frac{N}{2} - m}{N + 1}e^{-\Lambda_m^{\text{pop}}(t)}\right],$$
$$(56)$$

where

$$\Lambda_m^{\text{pop}}(t) = \frac{8A^2(N+1)}{\Omega_+^2(m)}\left(1 - \cos[\Omega_+(m)t]\right). \qquad (57)$$

As demonstrated in Fig. 5 this result gives an excellent approximation of the exact dynamics in the perturbative regime. For longer integration times, the position and the width of the revivals are reproduced very well, while
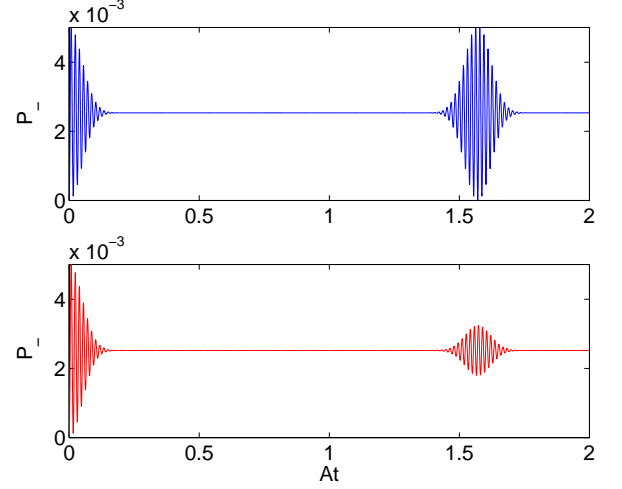

FIG. 6: (Color online) Population of the central spin according to the second-order TCL approximation (top) and to the exact solution (bottom). Parameters: $N = 101$ and $\alpha = 0.5$.

their height is not (see Fig. 6). We find again that the NZ result is hardly distinguishable from the corresponding TCL result, and hence refrain from showing it in a separate figure.

The standard procedure that uses the product-state projection operator (1) with $\rho_0 = 2^{-N}I_E$ yields the upper state population

$$P_+(t) = \frac{1}{2}\left[1 + \exp\left(-\frac{8A^2N}{\omega_0^2}(1 - \cos\omega_0 t)\right)\right], \quad (58)$$

which is also plotted in Fig. 5. We see that the standard projection operator technique leads to a rather bad approximation which is neither able to represent correctly the damping nor the revivals of the populations.

C. Complete projection onto the angular momentum manifolds

For the present model we can construct another correlated projection superoperator which takes into account both conserved quantities, namely J_3^{tot} and $\boldsymbol{J}^2$. This projection is given by

$$\mathcal{P}\rho = \sum_{jm}\text{tr}_E\{\Pi_{jm}\rho\}\otimes\frac{1}{N_j}\Pi_{jm} \equiv \sum_{jm}\rho_{jm}\otimes\frac{1}{N_j}\Pi_{jm},$$
$$(59)$$

where N_j has already been defined in Eq. (29). The Π_{jm} denote the ordinary projection operators that project onto the common eigenspaces of J_3 and $\boldsymbol{J}^2$ with corresponding eigenvalues m and $j(j + 1)$. The map (59) obviously leaves invariant J_3^{tot} and $\boldsymbol{J}^2$ and fulfills again all conditions formulated in Sec. II D.

The second-order NZ master equation corresponding

to the projection (59) reads

$$\frac{d}{dt}\rho_{jm}(t) = 4A^2 \int_0^t dt_1$$
$$\times \Big[\sigma_+ \rho_{j,m+1}(t_1)\sigma_- b(j,m) 2\cos[\Omega_+(m)(t-t_1)]$$
$$+ \sigma_- \rho_{j,m-1}(t_1)\sigma_+ b(j,-m) 2\cos[\Omega_-(m)(t-t_1)]$$
$$- \sigma_+\sigma_-\rho_{jm}(t_1)b(j,m)e^{i\Omega_+(m)(t-t_1)}$$
$$- \sigma_-\sigma_+\rho_{jm}(t_1)b(j,-m)e^{i\Omega_-(m)(t-t_1)}$$
$$- \rho_{jm}(t_1)\sigma_+\sigma_- b(j,m)e^{-i\Omega_+(m)(t-t_1)}$$
$$- \rho_{jm}(t_1)\sigma_-\sigma_+ b(j,-m)e^{-i\Omega_-(m)(t-t_1)}\Big], \quad (60)$$

where $b(j,m) = j(j+1) - m(m+1)$. Of course, the TCL version is obtained again by replacing $\rho_{jm}(t_1)$ with $\rho_{jm}(t)$ under the time integral.

The procedure for the determination of the coherences and the populations of the central spin is analogous to the one of the previous case. Again, we find that the NZ and the TCL approach yield similar results for the coherences. An example is shown in Fig. 7 for the TCL approximation only. We see that the second order with the projection (59) leads to an excellent approximation for the coherences even for very long integration times.
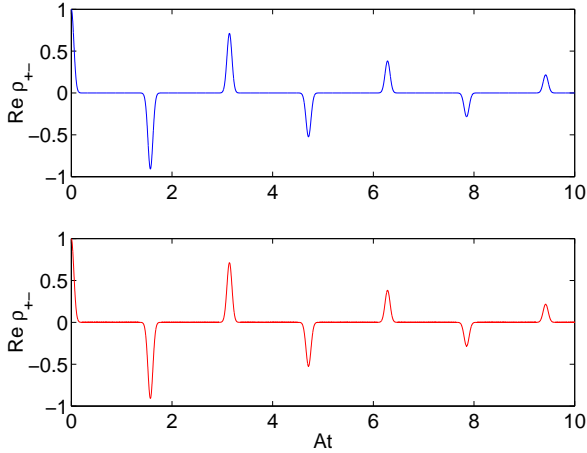

FIG. 7: (Color online) Coherence of the central spin. Top: Second-order TCL approximation for the projection (59). Bottom: Exact solution. Parameters: $N = 101$ and $\alpha = 0.1$.

A further remarkable feature of the projection (59) is that the corresponding NZ equation of second order (60) reproduces the *exact* dynamics of the populations. This can be demonstrated by solving the equations for the populations obtained from the master equation (60). Alternatively, we can prove this statement directly with the help of the following argument. We first note that by use of Eq. (5) the von Neumann equation (2) leads to the exact equation

$$\frac{d}{dt}\mathcal{P}\rho(t) = \int_0^t dt_1 \mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\rho(t_1), \quad (61)$$

from which we obtain an exact equation for the populations of the central spin:

$$\frac{d}{dt}\langle\pm|\mathcal{P}\rho(t)|\pm\rangle = \int_0^t dt_1 \langle\pm|\mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\rho(t_1)|\pm\rangle. \quad (62)$$

The crucial point is that for arbitrary $\rho(t_1)$ the following relation holds,

$$\langle\pm|\mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\rho(t_1)|\pm\rangle = \langle\pm|\mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{P}\rho(t_1)|\pm\rangle. \quad (63)$$

Hence, when calculating the diagonal elements of the density matrix we may insert at any time a factor of $\mathcal{P}$ in front of the density matrix $\rho(t_1)$. This fact is obviously related to the invariance of the subspaces spanned by the states $|+\rangle \otimes |j,m\rangle$ and $|-\rangle \otimes |j,m+1\rangle$, a fact that has already been used to solve the Schrödinger equation. For a formal proof one uses the expression (59) to demonstrate that Eq. (63) is a direct consequence of the relation

$$\mathcal{L}^\dagger(t_1)\mathcal{L}^\dagger(t)\left(|\pm\rangle\langle\pm| \otimes \Pi_{jm}\right) = \sum_{m'} A_{jm'} \otimes \Pi_{jm'} \quad (64)$$

with certain system operators $A_{jm'}$.

Using now the relation (63) in Eq. (62) we find

$$\frac{d}{dt}\langle\pm|\mathcal{P}\rho(t)|\pm\rangle = \int_0^t dt_1 \langle\pm|\mathcal{P}\mathcal{L}(t)\mathcal{L}(t_1)\mathcal{P}\rho(t_1)|\pm\rangle. \quad (65)$$

This equation is exact and coincides with the equation for the population that is obtained from the second-order NZ equation (6). We conclude that the NZ equation of second order indeed yields the exact dynamics of the populations.

IV. CONCLUSIONS

We have investigated the performance of the correlated projection operator method in the case of a spin-bath model where a central spin couples to a spin bath via full Heisenberg interaction. The coupling constants have been chosen to be uniform such that one can construct an exact solution of the von Neumann equation. We have considered two different projection superoperators, one of which projects onto the eigenspaces of the 3-component J_3 of the total bath angular momentum. The other projection operator projects onto the simultaneous eigenspaces of J_3 and the square $\boldsymbol{J}^2$ of the total bath angular momentum. The choice of these projections is motivated by the fact that both J_3^{tot} and $\boldsymbol{J}^2$ are conserved under the dynamics given by the full system Hamiltonian. The projection superoperators studied here thus fully exploit the known symmetries of the model, granting the invariance of the expectation values of the conserved quantities. For both projectors we have solved the Nakajima-Zwanzig and the time-convolutionless master equation to second order in the interaction and have compared the results to the exact solution.

Both the NZ and the TCL master equation lead to a relaxation and decoherence behavior that approximates the exact solution very well. Remarkably, also the position and the width of the partial revivals of the coherence and the populations could be reproduced. For all tested parameter sets, the TCL and NZ solutions were hardly distinguishable. In these cases the TCL approach is to be favored because of its much simpler structure.

A remarkable property of the projection superoperator that projects onto the simultaneous eigenspaces of $\boldsymbol{J}^2$ and J_3 is that the corresponding second-order NZ equation results in the exact dynamics for the populations. While the standard product state projection gives only a poor approximation, the above correlated projection reproduces the exact solution already in lowest order. This illustrates an important feature of the correlated projection operator method. Namely, different choices for the projection $\mathcal{P}$ yield dynamic equations of different structure for different sets of relevant variables. Therefore, the resulting expressions for the quantities of interest, e.g. the populations, may differ in all orders of the cou-

pling. Hence, changing the projection operator corresponds in general to a non-perturbative reorganization of the expansion for the desired quantities.

Finally, we emphasize that all calculations in this paper involving projection operator techniques can be carried out in a similar way for more realistic assumptions regarding the coupling constants. The correlated projection operator technique may thus be applicable to many physically relevant problems featuring non-Markovian dynamics, such as the hyperfine interaction of an electron confined to a quantum dot, the spin dynamics under a spin-echo pulse sequence, or the spin dynamics in a molecular magnet.

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[49] More precisely, these states should be written as $|j, m, \lambda\rangle$, where λ stands for additional quantum numbers which, together with j and m, uniquely fix the basis state.

[50] We use the convention that $\rho_{\frac{N}{2}+1} = \rho_{-\frac{N}{2}-1} = 0$.